Chlorthal-dimethyl

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.82e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.74e-01

Confidence level: 3.79e-01

Nearest Neighbors from the Training Set

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Trimethylethoxysilane
Measured: 2.50e-06
Predicted: 86.7

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Dimethametryn
Measured: 7.28e-06
Predicted: 1.60e-06

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1,1'-Biphenyl, (1-methylethyl)-
Measured: 4.05e-05
Predicted: 3.10e-03

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Fluthiacet-methyl
Measured: 4.95e-08
Predicted: 6.62e-09